UCRL-JC-148180

ENDF/B-VI Coupled Photon-Electron Data for Use in Radiation Shielding Applications

D. E. Cullen

February 15, 2002

U.S. Department of Energy

Lawrence
Livermore
National
Laboratory

This work was performed under the auspices of the U. S. Department of Energy by the University of California, Lawrence Livermore National Laboratory under Contract No. W-7405-Eng-48.

ENDF/B-VI Coupled Photon-Electron Data for Use in Radiation Shielding Applications

by

Dermott E. Cullen
University of California
Lawrence Livermore National Laboratory
L-128
Livermore, CA 94550

and

Robert E. MacFarlane
University of California
Los Alamos National Laboratory
MS B243
Los Alamos, NM 87545

an Invited Paper for presentation at the Twelfth Biennial Topical Meeting of the Radiation Protection and Shielding Division, of the American Nuclear Society, to be held April 14-17, 2002 in Santa Fe, New Mexico

This Paper will soon be available on-line at
http://www.llnl.gov/cullen1

Abstract

In radiation shielding applications we need photon and electron data, as well as computer codes that utilize these data, in order to predict results inexpensively and safely. In this paper we will first cover the current status of available photon and electron data that have only recently been adopted for inclusion in ENDF/B-VI, with emphasis on the improved detail that is included in these data bases. Next we will cover the availability of these data bases and computer codes that use them.

Introduction

In the last few years our photon and electron data bases have been greatly improved in terms of the detail included as well as the accuracy of the data. At the same time there has been an enormous increase in the availability of inexpensive computer power. The combination of improved photon and electron data bases and increased available inexpensive computer power allows us today to calculate results in greater detail, to greater accuracy, using the best methods, such as Monte Carlo, which was not practical just a few short years ago.

In this paper we will describe the current status of everything that we need in order to perform photon and electron radiation transport calculations. First we will cover the current status of available ENDF/B-VI photon and electron data, with emphasis on the improved detail that has only recently been added to our data bases. Next we will cover the availability of these data and computer codes that use them.

Photon and Electron Data Bases

We will discuss three different data bases:

1) The Evaluated Photon Data Library, ’97 Version (EPDL97) (ref. 1)

2) The Evaluated Electron Data Library (EEDL) (ref. 2)

3) The Evaluated Atomic Data Library (EADL) (ref. 3)

The Evaluated Photon Data Library (EPDL97) describes the interaction of photons with matter as well as the direct production of secondary photons and electrons. The Evaluated Electron Data Library (EEDL) describes the interaction of electrons with matter as well as the direct production of secondary electrons and photons. The Evaluated Atomic Data Library (EADL) describes the relaxation of atoms back to neutrality following an ionizing event, i.e., it describes the spectra of fluorescence photons from radiative transitions and electrons from non-radiative transitions as an ionized atom returns to neutrality.

These three libraries are designed to be used in combination to perform detailed coupled electron-photon radiation transport calculations. They all contain elemental data for Z = 1 through 100, over the energy range 10 eV to 100 GeV. They are all completely consistent with one another in terms of all using the same atomic parameters (e.g., subshell binding energies). These libraries include details that were not previously available to us, or not considered when performing calculations using what we will call traditional photon interaction data.

Traditional Photon Interaction Data

Traditionally, the data included in a photon interaction data base have been sufficient to describe the interaction of primary photons with matter. The data traditionally contained in this data base included,

1) Cross sections for coherent and incoherent scattering, pair production and photoelectric absorption.

2) Form factors and scattering functions, used to describe the angular distribution of coherent and incoherent scattered photons

Although these data are sufficient to describe the interaction of primary photons, they are not adequate to uniquely define the emission of secondary photons following photoelectric effects; e.g., fluorescence. These data also did not include the effect of anomalous scattering, which significantly affects coherent scattering near and below the photoelectric absorption edges. Lastly, these data did not differentiate between pair and triplet production.

Additional Photon Interaction Data

In addition to the data traditionally included, the EPDL97 data base now contains:

1) Cross sections for each photoelectric subshell, pair and triplet production cross sections, a coherent cross sections accounting for anomalous scattering.

2) Anomalous scattering factors, used in combination with form factors, to describe the angular distribution of coherently scattered photons.

To illustrate the increased detail that this library includes, Figure 1 shows the traditional lead photon cross sections. Essentially we need merely four types of cross sections to describe coherent and incoherent scattering, photoelectric absorption and pair production. Figure 2 illustrates the additional lead photoelectric subshell cross sections for 24 separate subshells.

Figure 3 illustrates the lead electron ionization subshell cross sections for the same 24 subshells included in the EEDL library. Is it important to have this additional detail?

Traditionally when a photoelectric event occurs all of the energy is assumed to be deposited at the point of the event. Figure 4 illustrates that in fact when a photon undergoes photoelectric absorption just above the K edge in lead, 87.9 % of the energy is re-emitted as fluorescence x-rays just below the K edge, where the cross section is much smaller than it is above the edge, allowing these x-rays to be quite penetrating.

From Figure 4 we can see that following a single K shell vacancy there is a shower of over one hundred fluorescence x-ray emission lines. Without photoelectric subshell cross sections and transition probabilities it is not possible to accurately define the probability of this fluorescence x-ray emission. Therefore having this detail is indeed important.

Is anomalous scattering important? From Figure 1 we can see that with anomalous scattering included the coherent scattering cross section at low energy is decreasing and near 10 eV in lead it is about 10 barns. In contrast, without including anomalous scattering it is about 4480 barns - a factor of 448 times too large! Only if you consider the difference between 10 and 4480 barns to be insignificant would you conclude that this is not an important effect.

Related Data Bases

EPDL97 is designed to be used with two of our other data bases to allow coupled photon-electron transport calculations in order to completely account for the emission of all secondary photons, as well as a more detailed description of energy, dose, etc. deposition within media. These two data bases include: 1) an electron interaction data base, covering the same range of elements (Z = 1 to 100) and energy range (10 eV to 100 GeV) as our photon interaction data base; 2) an atomic relaxation data base, to describe the relaxation of atoms back to neutrality following any ionizing event; during the relaxation, photons (fluorescence) and electrons can be emitted by the atom, which should be considered in a photon-electron calculation, or even in a basic photon transport calculation. Figure 3 above illustrates the lead electron ionization subshell cross sections contained in our electron interaction library. Figure 4 illustrates the radiative emission due to a vacancy in the K shell of lead. These results were calculated using our atomic relaxation data base EADL.

What's Missing

We have come a long way in the last few years toward being able to accurately model the transport of photons and electrons through matter, but we still aren't where we would like to be. For complete details of how our data bases could be improved see the EPDL97 documentation (ref. 1). Here we will mention only one thing that is still missing from our data bases, namely photonuclear data. Photonuclear reactions have some potentially very positive effects that we could utilize in our applications; e.g., they can cause strong, very localized energy deposition. They also have some potentially very negative effects, such as activating your accelerator. Suffice it to say that there are a wide variety of reasons why it would be desirable for us to have an accurate and generally available data base for photonuclear reactions.

There are a number of currently available radiation transport codes that use models to describe photonuclear reactions. However, as yet these data has not been systematically reduced to simple data bases for inclusion in ENDF/B-VI. Currently there is an effort under way to develop a data base of photonuclear reactions and hopefully in the not too distant future these data will be generally available. In particular it is worth mentioning the coordinated work between NJOY and MCNP; for the current status of this work see,
http://t2.lanl.gov/data/photonuclear.html.

Processing and Application Codes to Use this Data

It is very nice that we have these data bases, but without computer codes that actually process these data for use in applications, and then use these data in applications these data bases aren't of much practical use.

Processing Codes: NJOY

The NJOY Nuclear Data Processing System (ref.4) is widely used to convert data in the ENDF format into libraries for use in nuclear applications. Work is now underway to update NJOY to make use of the increased detail and accuracy of the atomic data libraries discussed here. Sometimes this work has to be coordinated with improvements in the applications. As an example, the MCNP Monte Carlo code currently uses a somewhat abbreviated representation of fluorescence, that simplifies the subshell structure. Interim libraries that use the existing fluorescence scheme with the more accurate modern cross sections are now under development.

Future improvements in NJOY processing and the MCNP formats and fluorescence schemes will allow for dramatic improvements in the predictions of such things as photon and electron spectra emitted from surfaces. Deterministic S_N codes often handle photon data by making use of coupled sets with different blocks of data for neutron-neutron, neutron-photon, and photon-photon effects. The new work now going on to standardize photonuclear data evaluations will soon allow us to fill in the photon-neutron block of a coupled set. The current multi-group libraries for deterministic transport treat photoionization as an absorption reaction. By making use of these new atomic data libraries in NJOY, we will be able to treat photoionization with both photons in and photons out (fluorescence), that is, as a part of the transfer matrix.

Monte Carlo Radiation Transport: TART

Although EPDL97 has only recently been adopted for inclusion in ENDF/B-VI, it has been used for years by TART, to provide modern, more accurate cross sections allowing greater detail for our photon applications; only in this way can we respond to the ever increasing depend for more accurate results.

Usually when Monte Carlo radiation transport is described, it is said that its big advantage is that it can be used to model arbitrary geometry, which is indeed true. However, what it often overlooked is its ability to also accurately model reaction kinematics, something that deterministic methods, such as S_N, have trouble doing. For example, the angular distributions for scattered photons and electrons are extremely anisotropic, which makes it very difficult to accurately model using deterministic methods. In contrast, this is no problem at all to accomplish using Monte Carlo, including complete correlation between scattering angle and secondary energy on a continuous energy basis.

This ability of Monte Carlo to more accurately model kinematics has allowed TART to take full advantage of the increased details now available in EPDL97. Only by incorporating this increased detail can our codes keep up with the even increasing demand for more accurate answers. Again, let me stress that this is only possible using Monte Carlo, which is why we see it used more often today. For more details on TART, see the on-line documentation at,
http://www.llnl.gov/cullen1

Conclusions

In this paper, we have described details of the EPDL97 photon interaction data base. This data base is designed to meet the needs of two different groups of users: 1) Those who would like to use these data in the traditional sense, without including additional details in the calculations - we have taken care to insure that this can still be done, and 2) Those who would like to extend their calculations to include more details in their photon (and if desired, coupled electron) transport calculations. Care has been taken to insure that EPDL97 can be used by either group of users.

The three data bases, EPDL97, EEDL, and EADL are documented in ref. 1, 2 and 3, NJOY in ref. 4, and TART is documented in ref. 5. All are currently available from data centers throughout the world. To obtain copies of documentation and for details of how to obtain these data bases see the website at http://www.llnl.gov/cullen1. EPDL97, EEDL and EADL are now available on-line in the ENDF/B-VI and ENDL formats from the IAEA, Vienna, at http://www-nds.iaea.org/epdl97. They are also available in an interpreted format at http://t2.lanl.gov/data/atomic.html.

References

1) D. E. Cullen, J. H. Hubbell, and L. Kissel, “EPDL97: the Evaluated Photon Data Library, '97 Version," UCRL-50400, Vol. 6, Rev. 5, Lawrence Livermore National Laboratory, Livermore, CA, (September 1997); now availanle on-line at,
http://www-nds.iaea.org/epdl97/

2) S. T. Perkins, D. E. Cullen and S. M. Seltzer, "Tables and Graphs of Electron-Interaction Cross Sections from 10 eV to 100 GeV Derived from the LLNL Evaluated Electron Data Library (EEDL), Z = 1-100," UCRL-50400, Vol. 31, Lawrence Livermore National Laboratory, Livermore, CA, (November 1991); now available on-line at,
http://www-nds.iaea.org/epdl97/

3) S. T. Perkins, et.al, "Tables and Graphs of Atomic Subshell and Relaxation Data Derived from the LLNL Evaluated Atomic Data Library (EADL), Z = 1-100," UCRL-50400, Vol. 30, Lawrence Livermore National Laboratory, Livermore, CA, (October 1991); now available on-line at,
http://www-nds.iaea.org/epdl97/

4) R.E.MacFarlane and D.W.Muir, “The NJOY Nuclear Data Processing System, Version 91”, Los Alamos National Laboratory report LA-12740-M (1994).

5) D. E. Cullen, “TART2000: A Coupled Neutron-Photon 3-D, Combinatorial Geometry Monte Carlo Transport Code”, UCRL-ID-126455, Rev. 3, Lawrence Livermore National Laboratory, Livermore,

CA, (November 2000).

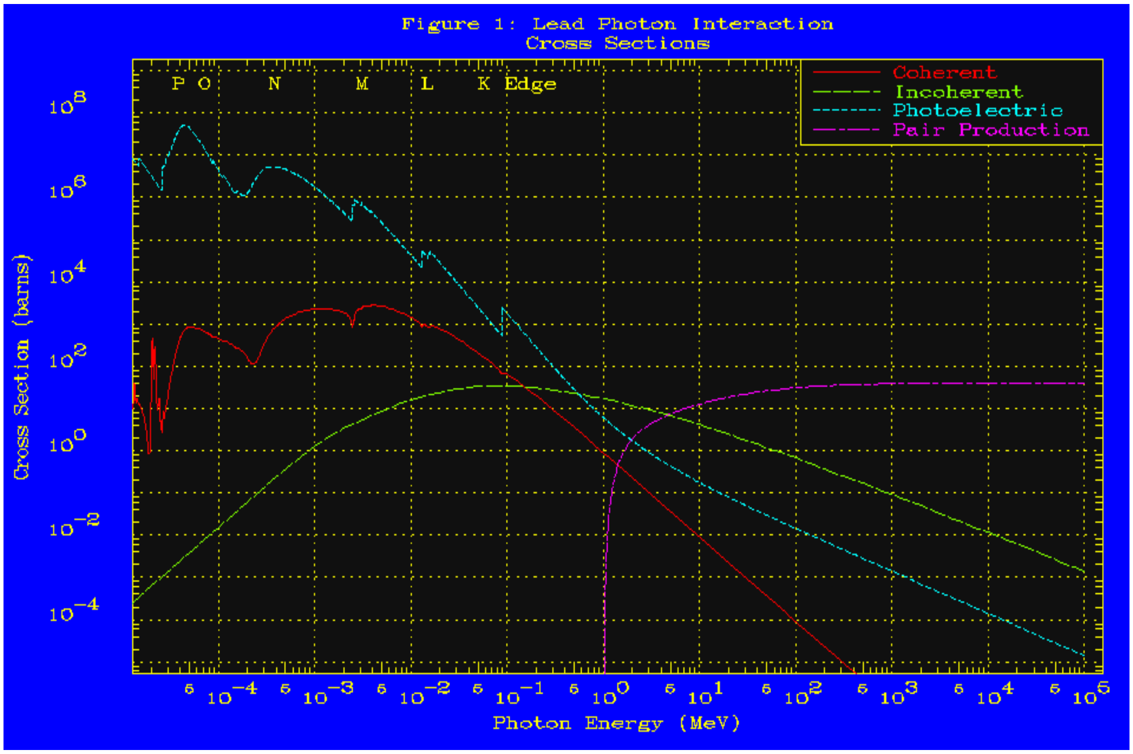

Fig. 1: Traditional lead photon cross sections

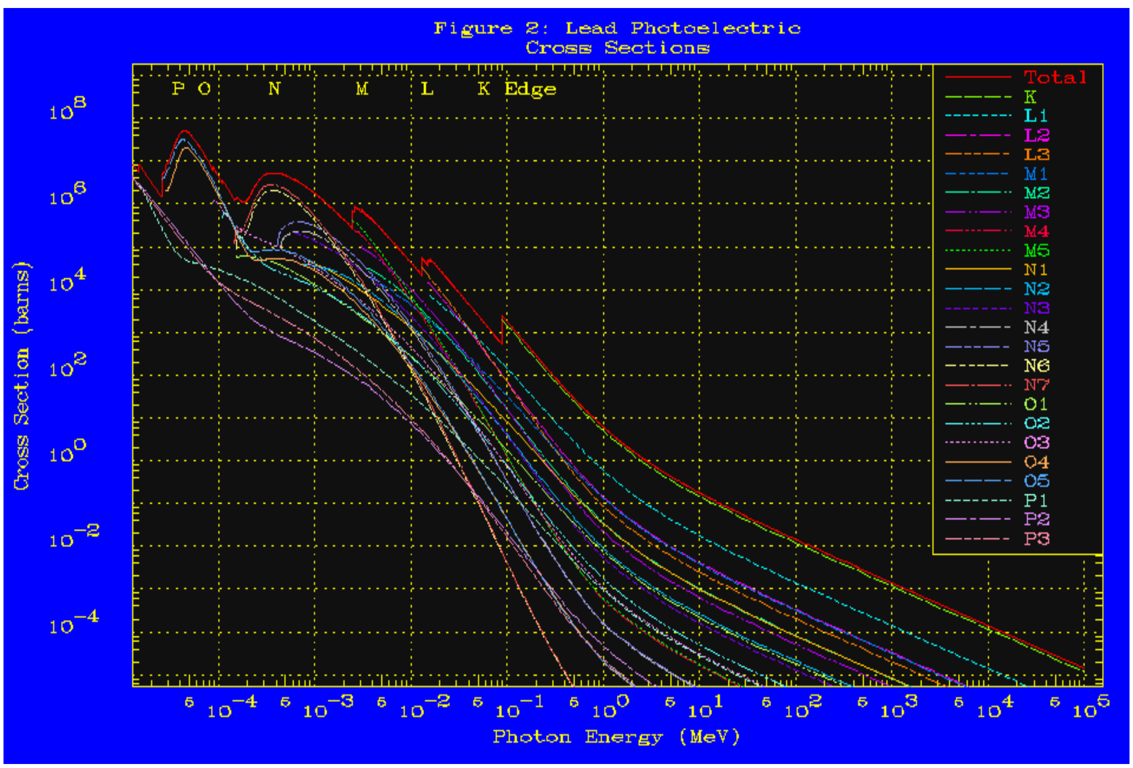

Fig. 2: Lead photoelectric subshell cross sections

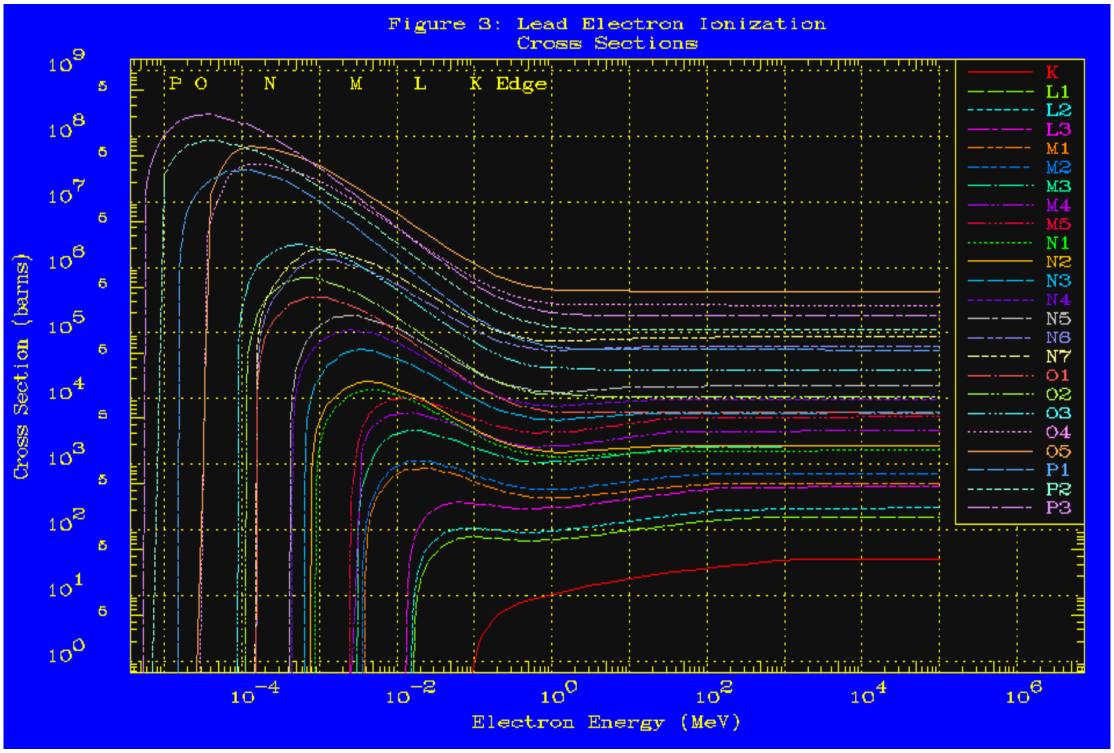

Fig. 3: Electron ionization cross sections

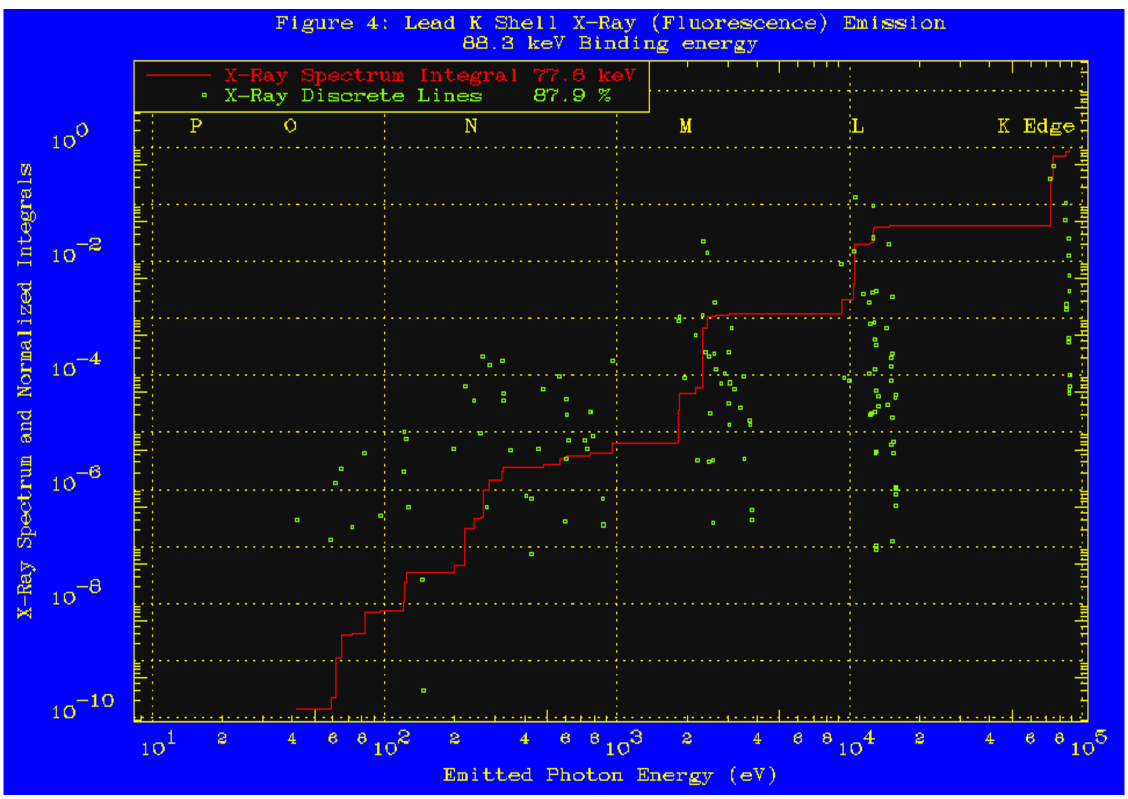

Fig. 4: Fluorescence emission due to a K shell ionization

University of California
Lawrence Livermore National Laboratory
Technical Information Department
Livermore, CA 94551